

AMENDMENT

Kindly amend the application, without prejudice, as follows:

In the abstract:

Rewrite the abstract to read as set forth on the attached separate sheet.

In the claims:

Rewrite claim 1 to read as follows:

- C1
Sub B1
1. (amended) A method for determining molecular crystal structures from powder diffraction data comprising the steps of:
- providing a powder diffraction pattern of a molecular crystal structure;
 - generating a reduced representation of the powder diffraction pattern in dependence on a predetermined unit cell and space group of the molecule under examination in which the total quantity of diffraction data is significantly reduced whilst maintaining the characteristics of the diffraction data that are representative of the crystal structure under examination;
 - determining a set of variables for describing trial molecular structures, derived from predetermined internal coordinates and said space group;
 - assigning values to said variables thereby creating a population of trial structures each defined by a unique set of values for said variables;
 - calculating a fitness for each trial structure with respect to the reduced representation of the powder diffraction pattern;
 - determining whether any one of the calculated fitnesses is less than or equal to a predetermined threshold;
 - where none of the calculated fitnesses is less than or equal to the threshold value, selecting at least one survivor from the population of trial structures, altering the values of the variables of at least one of the survivors in accordance with one or more predetermined rules, calculating the fitnesses of the new trial structures; and repeating the steps of selecting survivors, altering the values of the variables and calculating the fitnesses of the new trial structures until at least one of the calculated fitnesses is less than or equal to the threshold value, and

C¹ where at least one of the calculated fitnesses is less than or equal to the threshold,
outputting at least on trial molecular crystal structure represented by the successful sets of
values.
